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Computational Modelling of Multi-Physics and Multi-Scale Processes in Parallel

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This paper provides an overview of the developing needs for simulation software technologies for the computational modelling of problems that involve combinations of interactions amongst varying physical phenomena over a variety of time and space scales. Computational modelling of such problems requires software technologies that enable the mathematical description of the interacting physical phenomena together with the solution of the resulting suites of equations in a numerically consistent and compatible manner. This functionality requires the structuring of simulation modules for specific physical phenomena so that the coupling can be effectively represented. These *multi-physics* and *multi-scale* computations are very compute intensive and the simulation software must operate effectively in parallel if it is to be used in this context. An approach to these classes of multi-disciplinary simulation in parallel is described, with some key examples of application to challenging engineering problems.

Keywords Multi-Physics, Multi-Scale, Parallel, Casting, Granular Flow

1. INTRODUCTION

As we move into a new generation of escalating pressures, in respect to shortening time-scales in the design and manufacturing cycles, the role of simulation will become increasingly central to the whole virtual engineering venture. However, to represent sufficiently and comprehensively the behavior of engineering processes requires simulation capabilities that capture both:

- the interactions amongst continuum phenomena at the macro-scale, i.e.multi-physics, and
- the impact of behavior across a range of length and time scales simultaneously, i.e. multi-scale.

Mathematically, the representation of the impact of one physical phenomenon, e.g. temperature, on another, e.g. fluid flow, is enabled by either a local condition at the boundaries of a sub-domain of the whole physical solution domain or through a source term body load, e.g. a force, over part of the solution domain. This means that computational models of closely coupled multi-physics require the numerical solution procedures of all the phenomena to have a measure of compatibility, so that the impact of one of the phenomena, e.g. electro-magnetic field, can be represented in another, e.g. fluid flow, in a time- and space-accurate manner. Moreover, when multi-scale calculations are involved, a variety of domain decomposition techniques are utilised, which again require a measure of compatibility amongst the computational solvers for the phenomena at each of the scales. Multi-physics and multi-scale calculations are very computationally intensive, so that the simulation tools targeted at such applications will have to exploit high performance parallel computing (HPPC) systems. To effectively exploit HPPC systems, these heterogeneous applications must be structured in parallel so that they are load balanced upon heterogeneous computing systems as exemplified by HPPC clusters. This paper gives an overview of the multi-physics and multi-scale simulation challenges and describes one approach to addressing the arising issues. This overview is illustrated through a variety of complex simulation challenges that demonstrate the issues discussed.

2. SIMULATION STRATEGIES FOR MULTI-PHYSICS MODELLING

At the macro-scale the equations of continuum physics serve to describe the phenomena that are active in a process or system. Multi-physics modelling summarizes the class of problems

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that involve the interaction amongst some or all of these continuum phenomena, i.e. fluid flows, heat transfer, solid mechanics, electro-magnetics and acoustics. This means that the sets of equations for each of the specific phenomena have to be coupled in some way. This coupling can vary in its strength—the stronger it is, the more complex and non-linear the solution process becomes. Of course, each of the solution strategies for each of the phenomena must involve a discretization of the physical domain using typically either finite element (FE) or finite volume (FV) solution-based procedures. However, it is quite possible that the solution strategy for each phenomenon might involve distinctive:

- mesh structures,
- mathematical approaches for the discretization of the physical phenomenon under consideration over the specified mesh structure,
- procedures for the solution of each of the equation sets governing each specific phenomena,
- direct and iterative linear solvers and possible consequent impacts upon the phenomena specific solution strategies.

For example, with regard to the computational solution of specific phenomena, the equations are typically solved in Eulerian or Lagrangian form; some solver strategies involve an assembly of the discretized equations into one large matrix and their global solution. For others, the strategy involves a procedure whereby the coupled equations defining one phenomenon, as in fluid flow, for example, are never fully assembled, but are partially solved and iterated to a solution. Hence, when attempting multi-physics simulation, incorporation of the physical coupling through the mathematical models has to negotiate a range of potential distinctions in the solution strategy for each of the phenomena involved:

- Mesh type, order and distribution,
- Eulerian or Lagrangian approach in the solution strategy,
- Method of discretization,
- Fully assembled or iterative segregated solver approach,
- Parallelization approach.

At this stage of computational mechanics modelling, most phenomena are solved with a specific approach that is embedded within a single piece of software that has often been optimized in a variety of ways to provide fast and accurate solutions. This software usually enables the user to add a series of problem specific configurations of the physical phenomena, material properties, geometries and boundary conditions. Typical examples here include tools such as ANSYS [1], NASTRAN [2], and ABAQUS [3] for problems rooted in solid mechanics, and CFX [4], FLUENT [5], and STAR-CD [6] for problems based in fluid mechanics. Both of these families of tools can handle thermal and a limited set of electric/magnetic problems. As such, if the coupling is one way and essentially weak, then it is possible to use the output from one phenomenon specific code, say code A, and map it into a mesh space that is suitable for incorporating relevant boundary conditions or volume loads into the code embedding the other phenomenon specific code, say code B. The physical information distributed over the mesh in code A has to be filtered and mapped into the mesh approximation structure of code B either throughout the volume or across the surface of a boundary within the solution domain of code B. This weak coupling means that the phenomenon represented in code A will converge in the normal fashion and code B will simply work with the boundary conditions or volume loads from code A to reach a converged solution. If the information provided by code A is well behaved, e.g. not varying too rapidly, and the mapping is suitably precise, then code B should converge reasonably well. However, if the information from code A is varying rapidly in space and or time and/or if the stability of the solver matrix systems in code B are very sensitive to this data, then this may impact adversely upon the solution performance of code B. This coupling is made more difficult when, for example, i) mesh structures are different, ii) one solution approach is Lagrangian and the other Eulerian, and/or iii) the solver strategies are distinctive, e.g. one is based upon a fully assembled matrix structure and the other is based upon an iterative segregated solver strategy. In principle, one can apply the reverse procedure to couple back the boundary or volume loads from code B to code A through the inverse mapping process from mesh to A to B. However, the numerical efficacy of this process is dependent upon all the same limitations as going from code A to B. As such, the development of a fully converged solution to strongly coupled physics can be a real challenge. Indeed, the physical coupling may well have to be weakened, in the mathematical sense, to reach a solution at all. This is generally the case, for example, in the representation of fluid-structure interaction in most industry standard aircraft flutter analyses.

In the last couple of years there have been some projects targeted at creating tools to facilitate the coupling of very distinct codes. Some projects include:

- MDICE a US Air Force funded project to develop a distributed integrated computing environment led by CFDR [7].
- ICE a US Army funded project targeted at coupled multi-disciplinary simulation across a GRID environment [8].
- MpCCI an EU funded project to develop a suite of tools to enable the coupling of a wide variety of commercial codes [9].

Of these, the last has begun to be used in the European context and examples of loosely coupled simulations are now emerging, modelling fluid-structure interaction with commercial computational fluid dynamics (CFD) and computational solid mechanics (CSM) codes, using FV and FE techniques, respectively. How well such an approach will model more closely coupled problems remains to be seen, especially for large problems when

TABLE 1
Definition of terms in generic transport equation

Phenomenon	ϕ	τ	Q_s	Γ_ϕ	Q_v
Continuity	1	1	$\rho\,\underline{v}$	0	S_{mass}
Velocity	$\underline{v}$	1	$\rho\,\underline{v}\underline{v}$	μ	$(S + \underline{J} \times \underline{B} - \nabla\rho)$
Heat transfer	h	1	$\rho\underline{v}h$	$\frac{k}{c}$	S_h
Electro-magnetic field	$\underline{B}$	1	$\underline{v}\underline{B}$	η	$(\underline{B}\nabla)\underline{v}$
Solid mechanics	$\underline{u}$	$\frac{\partial}{\partial t}$	$\mu(\nabla\underline{u})^T + \lambda(\nabla\cdot\underline{u} - (2\mu + 3\lambda)\alpha T)\underline{I}$	μ	$\rho\,\underline{f}_b$

the applications are almost certainly going to have to be run on high performance parallel systems. Another approach to the simulation of closely coupled interactions is described below.

3. CLOSELY COUPLED MULTI-PHYSICS SIMULATION IN PARALLEL

From the above discussion it is clear that if closely coupled multi-physics problems are to be modelled effectively using computational software, then the solution procedures for each of the specific phenomena should be compatible with respect to:

- The similarity of their mesh structure so that they can operate on essentially the same mesh (or its sub-sets) in order to facilitate the accurate exchange of coupling volume source and boundary data between solution procedures for each phenomenon.
- The compatibility of their solution strategy in a generally iterative context to enable the coupling of volume source and boundary data, especially in time varying problems.
- If, as in the case of fluid-structure interaction, the Eulerian and Lagrangian solution procedures are coupled this must be done with great care.
- The solution procedures must enable each phenomenon to be partitioned and load balanced in order to exchange information in an appropriate manner such that interprocessor communication does not compromise parallel scalability.

One attempt at building a software environment targeted at multi-physics simulation has been developed by the authors and their colleagues at the University of Greenwich. The PHYSICA software environment [10, 11] was originally targeted at the simulation of melting and solidification processes, and its key features are highlighted below. However, it would be remiss not to refer the reader to a range of other tools that have emerged over the last few years and are targeted at facilitating the solution of problems involving the interactions amongst continuum physical phenomena, see for example, FEMLAB [12], Oofelie [13], FOAM [14], RADIOSS [15] and the AUTODYNE series of codes [16], amongst others.

3.1. Generic Models and Computational Procedures

Especially in the context of solidification processing the following continuum phenomena and their interactions are of key significance:

- Free surface transient Navier Stokes fluid flow,
- Heat transfer by convection, conduction and radiation,
- Solidification/melting phase change,
- Non-linear solid mechanics, and possibly,
- Electro-magnetic forces.

It is useful to observe that all the above continuum phenomena can be written in the single form:

$$\frac{\partial}{\partial t}\int_v \rho\tau\phi\,dv + \int_s \underline{Q}_s\cdot\underline{n}\,ds = \int_s \Gamma_\phi\nabla\phi\cdot\underline{n}\,ds + \int_v Q_v\,dv \tag{1}$$

Table 1 provides a summary of the terms required to represent equation 1 for each of the above phenomena [11], where ρ is density, $\underline{v}$ is velocity, $\underline{S}$ is the source term, μ is viscosity, $\underline{J}$ is current, $\underline{B}$ is magnetic flux density, h is enthalpy, k thermal conductivity, c is specific heat, $\underline{u}$ is displacement, $\underline{f}_b$ is body force, α is the linear thermal expansion coefficient and T is temperature. For solid mechanics λ and μ are the Lame constants related to Young's modulus E and Poisson's ratio ν by:

$$\lambda = \frac{\nu E}{(1+\nu)(1-2\nu)} \quad \text{and} \quad \mu = \frac{E}{2(1+\nu)}$$

The suite of solution procedures chosen for the work outlined is based upon an extension of FV techniques from structured to unstructured meshes. The mesh structure is based upon low order approximations with arbitrary mixtures of tetrahedral, wedge, and hexahedral elements. Two forms of discretization are employed, with nodes located at either the center or the vertex of the element. This means control volumes can be constructed locally with reference to each element center or cell vertex, as illustrated in 2D in Figure 1. As such, the solution procedures can be based upon locally conceived solution procedures on mixed mesh structures and even though distinct discretization procedures may be used for different phenomena, this still enables

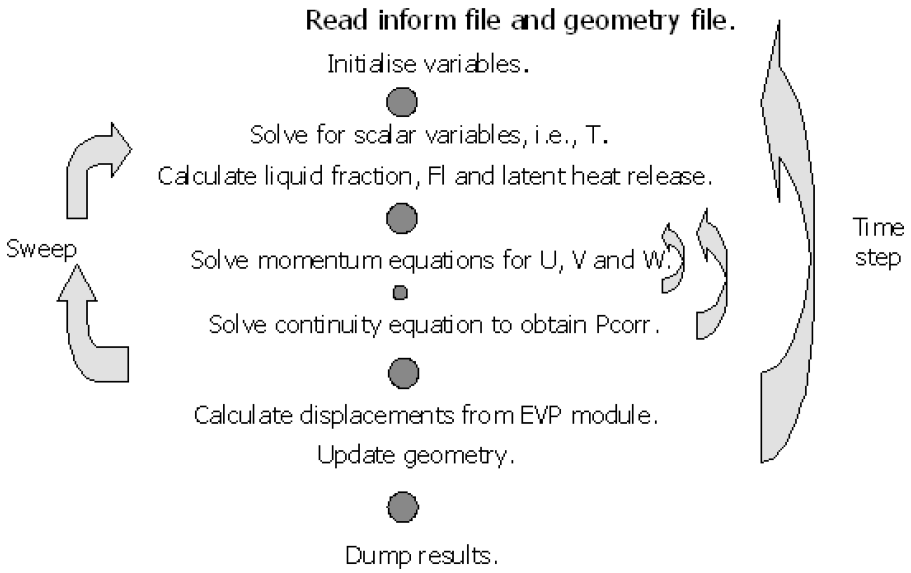

FIG. 1. Solution procedure for modelling solidification/melting.

the accurate mapping of volume and boundary source data from one procedure to another.

In this work, the fluid flow and heat transfer [17,18], chemical reactions [18,19] phase change [20] and electro-magnetics [21] procedures are based upon cell centred approximations, where the control volume is the element itself. However, McBride [22,23] has recently described in detail and evaluated the performance of some mixed approximation approaches for CFD following a vertex based strategy. The solid mechanics algorithms used in this work [24–26] employ a vertex based approximation, so that the control volume is assembled from components of the neighboring cells/elements to a vertex. Slone et al. [27] have also added a FE option to the solid mechanics using exactly the same mesh and solver strategy as for the FV methods, only the discretization approach has been altered, and the computational performance has been evaluated. The cell centered phenomena are all solved as an extension of the conventional SIMPLE pressure correction procedures for fluid flow originated by Patankar and Spalding [28]. Of course, with a cell centered co-located flow scheme, the Rhie-Chow approximation is used to prevent checker-boarding of the pressure field [29]. The pressure field is solved for using a simple diagonally pre-conditioned conjugate gradient method whilst the momentum fields are solved for with a simple SOR-like updating scheme. The solid mechanics solution procedure involves a formulation that leads to a linear system in displacement and is solved using a pre-conditioned BiCG technique, in a similar manner to finite element methods [26]. These FV procedures have been extended to model a range of nonlinear behavior [25].

The composite multi-physics solution procedure for solidification/melting processes, without electro-magnetic fields, for example, is highlighted in Figure 1. At this stage, a cautious approach to the solution strategy has been explored. If a phenomenon is not active in a cell or element, then it essentially skips any evaluation or computational work. This approach is important for simulating solidification/melting processes because, as phase change fronts move through the domain, the local "cocktail of physics" changes with time. Hence, passing across the whole mesh for each phenomena solver and for each time step is essential.

3.2. Design of a Multi-Physics Modelling Software Framework

The core technology embedded in the multi-physics modelling software environment is a three-dimensional code structure that provides an unstructured mesh framework for the solution of any set of coupled partial differential equations up to a second order [11]. The design concept is as object oriented as possible within the constraints of FORTRAN77. The challenge has been to build a multi-level toolkit that enables the modeller to focus upon the high level process of model implementation and assessment, and to simultaneously exert maximum direct control over all aspects of the numerical discretization and solution procedures.

The object orientation is essentially achieved through the concept of the mesh as constructed of a hierarchy of objects—nodes, edges, faces, volumes. Once the memory manager has been designed as an object hierarchy, all other aspects of the discretization and solution procedures can be related to these objects. This enables the software to be structured in a highly modular fashion, and leads to four levels of abstraction: the Model level, where the User implements the multi-physics models; the Control level, which provides a generic equation, for exploitation by the User, and solution control strategies; the Algorithm level, a whole set of tools for discretization, interpolation, source

construction, managing convection and diffusion, properties, system matrix construction, linear solvers, etc.; and the Utility level, file input-output tools for interaction with CAD software, memory manager, database manager, etc.

With the above abstraction framework it is quite possible to implement discretization and solution procedures to analyze distinct continuum phenomena in a consistent, compatible manner that particularly facilitates interactions. The current version of the multi-physics modelling software framework, PHYSICA has a) tetrahedral, wedge and hexahedral cell/element shapes, b) full adaptivity implemented in the data structures which are consistent for mesh refinement/coarsening and c) a range of linear solvers. It has the following core models:

- Single phase transient compressible free surface Navier-Stokes flow with a variety of turbulence models,
- Convection-conduction heat transfer with solidification/melting phase change, reaction kinetics and radiation,
- Elasto-visco-plastic solid mechanics,
- Electro-magnetics,

and their interactions.

3.3. The Parallelization Strategy

The use of a Single Process Multiple Data (SPMD) strategy employing mesh partitioning is now standard for CFD and related codes, see for example the Parallel CFD Proceedings [30]. Of course, when the code uses an unstructured mesh, the partitioning task is substantial. In this work the JOSTLE mesh partitioning and dynamic load-balancing tool [31, 32] has been employed. However, a key additional difficulty with respect to multi-physics simulation tools for solidification/melting problems is that the computational workload per node/mesh element is not constant.

In metals casting, for example, hot liquid metal fills a mold, and then cools and solidifies [33]. The liquid metal may also be stirred by electro-magnetic fields to control the metallic structure. This problem has many complexities from a load balancing perspective:

- At the start of the simulation the flow domain is full of air, which is expelled as the metal enters the domain. The resulting air-metal free surface calculation is more computationally demanding than the rest of the flow field evaluation in either the air or metal sub-domains.
- The metal loses heat from the moment it enters the mold and eventually begins to solidify.
- The mold is being dynamically thermally loaded and the structure responds to this.
- The electro-magnetic field, if present, is active over the whole domain.

The casting problem above has three sub-domains, which each have their own set of physics; however, one of these set of physics, the flow field, has a dynamically varying load throughout its sub-domain, and two of the sub-domains vary dynamically. If the solidified metal is an elasto-visco-plastic material its behavior is also non-homogeneous in compute terms.

As the approach employed here to the solution of multi-physics problems uses segregated procedures, in the context of iterative loops, it is attractive to take the approach of formulating the numerical strategy so that the whole set of equations can be structured into one large non-linear matrix. However, at this exploratory stage of multi-physics algorithm development, a more cautious strategy has been followed, building upon tried and tested single discipline strategies, for flow, structures, etc., and representing the coupling through source terms, loads, etc. An added complication here is that separate physics procedures may use differing discretization schemes. For example, in PHYSICA the flow procedure is cell centered, whilst the structure procedure is vertex centered. Of course, the load balancing problem that arises from multi-physics simulation is very challenging, as Hendrickson and Devine [33] point out in their review of mesh partitioning/dynamic load balancing techniques from a computational mechanics perspective. However, the JOSTLE toolkit developed at Greenwich has the key properties necessary to facilitate multi-physics load balanced simulation and is employed here [31, 32].

Finally, the parallelization strategy here [34] employs a message passing approach. It uses a generic thin layer message passing library, CAPLib [35], which maps onto PVM, MPI and Shmem, amongst others. CAPLib is targeted at computational mechanics codes and provides a compact data model that is very straightforward to apply. There is no measurable overhead in using CAPLib over the native message passing libraries [35].

4. MULTI-PHYSICS AND MULTI-SCALE APPLICATIONS

In the above sections an approach to the development of a core technology for the computational modelling of interacting continuum phenomena has been described. In this short overview there is only space to describe one example of each of the target multi-physics and multi-scale problem classes; however, the problems chosen reflect a series of generic issues that are important to highlight as challenges.

4.1. DC Casting of Aluminium Ingots

Direct Chill (DC) casting is a semi-continuous process widely used in the production of ingots by the aluminium industry. A schematic of the DC casting process geometry is given in Figure 2. Metal is poured into an open rectangular mold over a movable drawing block. As this drawing block moves downwards the metal is cooled first by contact with the mold and secondly by water sprays. During processing the ingot is subject to many distortions that arise as a consequence of combined thermal and mechanical effects. The deformation of the ingot walls may result in gap formation with the mold and this will impact adversely upon the cooling of the ingot as it forms. Thus the process is governed by a series of interacting phenomena,

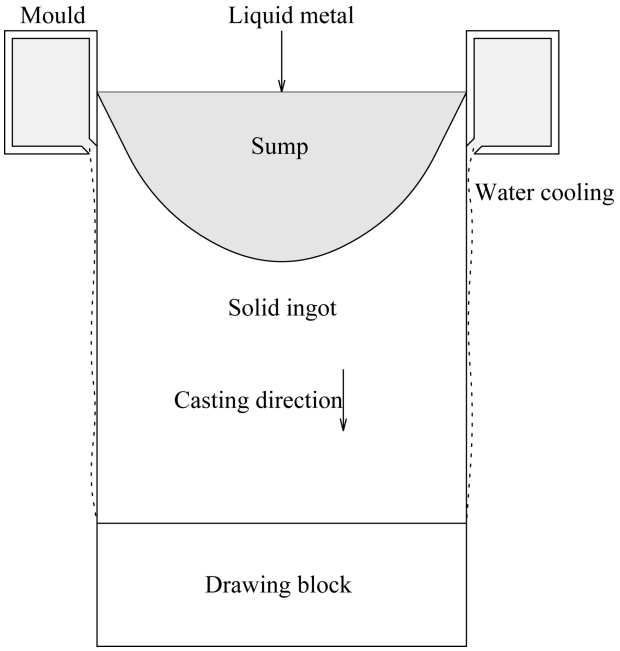

FIG. 2. Schematic of the DC casting process.

which include:

- Navier-Stokes free surface flow in the liquid region of the ingot,
- Heat transfer from the metal to the mould,
- Solidification of the alloy, and
- The development of stress and deformation in the cooling ingot.

Given that the injection rate of liquid metal can be balanced by the withdrawal rate of the drawing block, the top liquid metal surface is relatively stable and it may be assumed as fixed, which simplifies the CFD part of the calculation. With this simplification the above phenomena were solved simultaneously using the above multi-physics modelling environment. The flow was modelled by the Navier-Stokes equation, the solidification assumed a linear relationship between the temperature field and fraction solid, and the solid mechanics model assumed an elasto-visco-plastic material. The transient growth of the ingot domain is represented by a single mesh, which is initially compressed in the vertical direction. The mesh is subsequently stretched to match the rate of movement of the drawing block (see Figure 3). The mesh consists of 20560 hexahedral elements and 23241 nodes. The casting speed was .001 ms^{-1} and the time step was 5 seconds with a total simulation time of 1500 seconds. A detailed description of this DC casting model is given in Williams et al. [36, 37].

TABLE 2
Run times and speedup for the DC casting simulation on an Itanium cluster

P	t_{calc}	t_{file}	t_{total}	Sp_{calc}	t_{total}/t_{file}	$Sp_{overall}$
1	15316	23	15339	1	666.91	1
2	7079	65	7144	2.16	109.91	2.15
4	3582	98	3680	4.28	37.55	4.17
8	1902	131	2033	8.05	15.52	7.55
12	1448	154	1602	10.58	10.40	9.57
16	1166	161	1327	13.14	8.24	11.56

Samples of the simulation results are shown in Figures 4 and 5. The former shows the distribution of the thermal contours as the ingot grows from 500 to 1500 seconds. Figure 5 shows a cross section of the flow pattern in the liquid domain, the solidification degree and effective stress distribution at 1500 seconds.

The geometry in DC casting simulation is relatively simple, but the growth of the mesh with time adds another level of difficulty into the already complex physics problem. Table 2

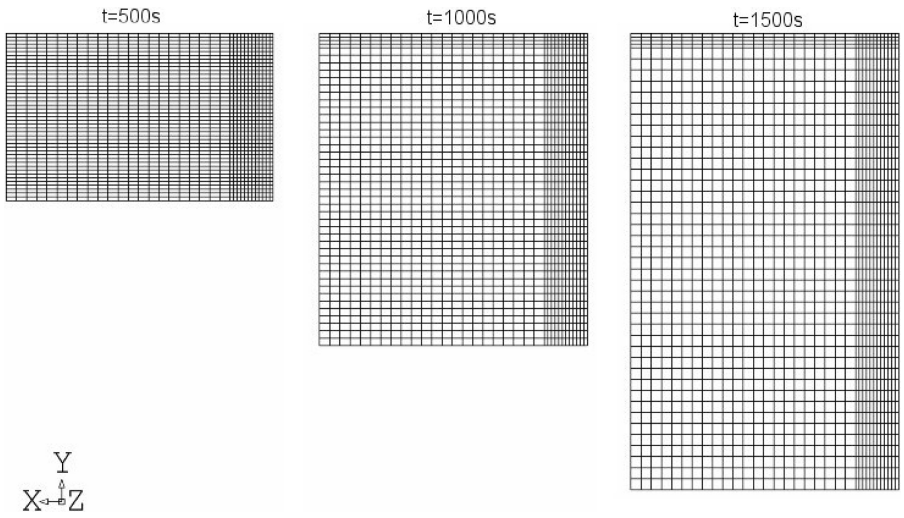

FIG. 3. Expansion of the mesh representing growth of the DC cast ingot.

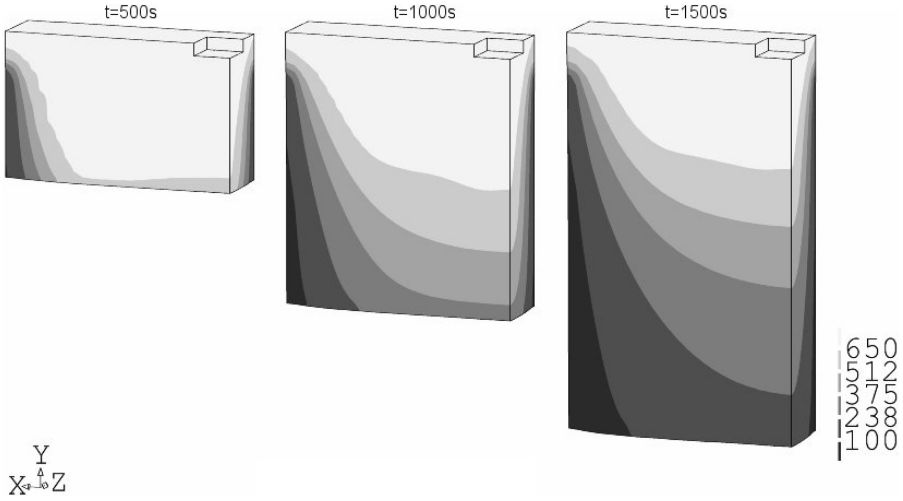

FIG. 4. Temperature contours (°C) at $t = 500$, 1000 and 1500 secs.

summarizes the parallel performance results, when the mesh has been partitioned as a homogeneous domain. The parallel scalability as represented by the speed-up based upon the compute calculation performance, though good, is poorer than for more homogeneous CFD problems, for example, and this is almost certainly caused by the additional calculations associated with the expanding mesh, as much as the modest mesh size. On this system, the overhead of reading and writing data to file has not seriously compromized the performance of the parallel calculations, though it almost certainly will do by the time 64 processors are employed for this problem size.

4.2. Multi-Scale Processes—Granular Flows

There are a large number of important processes in the context of engineering analysis where there are a range of time and length scales operating simultaneously. In this context it is neither computationally practical nor often necessary to represent the phenomena at the finest level in the detail of the macro-continuum scale. There are a number of ways of capturing the effects of the finest scale phenomena within the largest scale physics involved in a system. At some level all approaches involve defining a representative elementary volume (REV) to capture the scale of the phenomena at the finest length and time scales. Within the REV the physical behavior is assumed to be homogeneous, or well mixed, in space and to enable an integration of the physics effects in time. Amongst others, Voller [38] has described for example an approach to capturing most of the length scale range involved in metals solidification processes and Bennett et al. [39] has integrated the impact of the reaction of small particles within very large packed bed heaps.

For the sake of brevity the behavior of granular materials flowing into and out of storage devices, such as hoppers, will be considered, as they are an important feature in the processing of particulate solids in many industry sectors. Computational modelling of the flow of granular materials is complex because in reality the materials are an assembly of discrete particulates. Granular dynamics and micro-physical models are able to describe successfully the flow of granular material by accounting for particle-particle interactions at the microscopic level [40]. These models are effectively solved for using a computational approach based upon discrete element methods (DEM) [40,41].

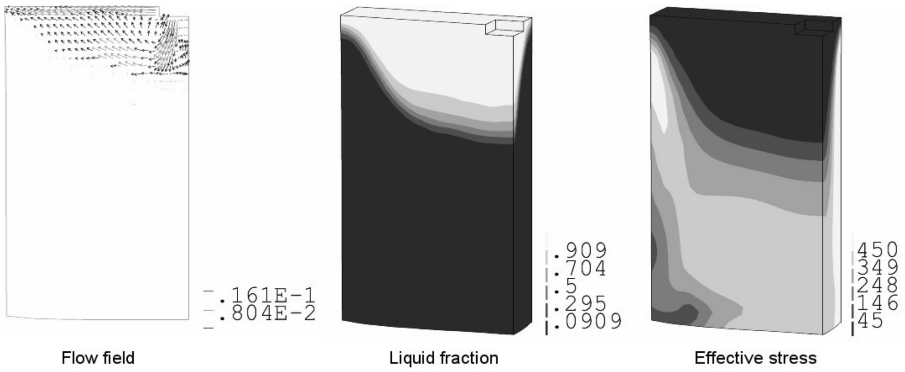

FIG. 5. Velocity, liquid fraction and effective stress in DC casting ingot.

In the last few years, Cleary et al. [42,43], amongst others, have attempted to use DEM to simulate full scale processes; these simulations involve from 100,000 to over one million particles and require many hours of compute time. In reality this means that for a simple hopper with a diameter of 5 m and a height of 7 m holding a granular material with an average diameter of 1 cm each one of the particles in the simulation would be representing the behavior of approximately 1000 real ones. Thus there are serious questions about how the DEM is tuned to capture the ensemble behavior of a cluster of granular particles as they move through the full scale vessel. This calls into question the suitability of such models for large-scale process modelling, as they would involve the simulation of the interaction of billions of particles—a time cannot be foreseen when this would be computationally practical. Hence, for all practical purposes the flow behavior must be modelled as a continuum [44, 45]. Although continuum models are partially successful in capturing some characteristics of the flow, they lack essential information on material parameters, which are needed to account for the interactions between different particles. Thus, their ability is limited in attempts to simulate some of the processes of significance in the process engineering industry, i.e. hopper filling/emptying, pneumatic conveying, etc., where, for example, particle-particle interactions might lead to phenomena such as particle size segregation.

However, it is possible to use micro-mechanical DEM based models to capture the behavior of multi-component granular mixtures and to both provide the form of and parameters for constitutive equations for the granular flows. This has been done in the QPM project [46, 47]. The granular material is assumed to flow as a conventional transport equation. However, the characteristics of the granular material are parameterized using information provided by DEM simulations on a relatively small assembly of particles subject to a wide range of operational scenarios.

In the transport equations, described by equation 1 and Table 1, the density ρ and viscosity μ are represented as mixtures and where ρ_{gran} and μ_{gran} are the granular solids density and pseudo-viscosity, resulting from the material properties of the individual mixture components. The scalar parameter f represents the fractional volume of total material present in a computational control-volume, total solids fraction, and results from the summation of all fractions of the individual material components f_i, typically defined by size, present in the control-volume. The scalar parameters f_i take values between 0, i.e. control volume empty of material component i and the maximum allowed packing fraction, always less than unity. The maximum allowed packing fraction is a function of the individual components' shapes, sizes, etc., and is taken as a model input value, determined through experimental data. There are a number of granular models, which connect the pseudo-viscosity, μ_{gran} to local stresses, velocity gradients, material bulk density, etc. [48]. However, for the simulations performed below and comparisons with experimental data, the pseudo-viscosity was evaluated via an initial calibration of the model to the material flow rate during discharge, a parameter that can be directly calculated in the micro-physical framework using DEM techniques, [41, 44–49]. Special consideration was given to appropriate initial/boundary conditions to determine the initial state of granular material that has been resting in bins and hoppers before discharge. The calculation of each of the individual material components f_i in a control volume was performed through the solution of transport equations, which, in the absence of sinks and sources, may be written as:

$$\frac{\partial f_i}{\partial t} + \nabla \cdot \left(f_i \underline{u}^b + J_i^{\text{seg}} \right) = 0 \tag{2}$$

where $\underline{u}^b$ is the bulk velocity vector and J_i^{seg} is a drift flux, which represents segregation of component i. The term J_i^{seg} is very important, since it dictates the motion of the individual species in the bulk and determines the levels of segregation in the mixture, see Christakis et al. [44, 45] for more details. Summation of all individual fractions in a control volume of the computational domain gives the total solids fraction f. A number of numerical schemes have been implemented and tested for the solution of equation 2 [46, 47]. In this work a Total Variation Diminishing (TVD) scheme proved to be the most robust and represented more accurately the segregation levels of the mixtures studied. The scheme was used within the context of the Scalar Equation Algorithm (SEA) [50] for the solution of the species transport equations for these simulations.

The segregation flux was analyzed in the micro-physical framework, by using principles of kinetic theory [48]. Starting from the reduced Liouville equation, a generalized Boltzmann equation that included inelastic collision effects was derived by considering conditions for particle chaotic motions. Thus, the non-equilibrium velocity distribution functions were determined for each particle size in a multi-component granular mixture through the use of a generalized Grad moment method. Particle drift velocities were derived and the segregation flux J_i^{seg} in equation 2 was expressed as:

$$J_i^{seg} = f_i \left(\underline{v}_i^D + \underline{v}_i^S + \underline{v}_i^P \right) \tag{3}$$

where $\underline{v}_i^D$ is the drift velocity of the ith material component due to diffusion, i.e. flow down the ith component fraction gradient, $\underline{v}_i^S$ is the drift velocity of the ith material component due to shear-induced segregation, i.e. the flow of coarser particles in the mixture across gradients of bulk velocity and $\underline{v}_i^P$ is the drift velocity of the ith material component due to gravity driven spontaneous percolation of the fines in a mixture through the coarse phase and it depends primarily on the available void spaces in the coarse phase matrix through which the fines can pass.

Functional forms were extracted for the drift velocities of equation 3. This work concentrated on the study of binary mixtures consisting of fines and coarse phases of equal densities.

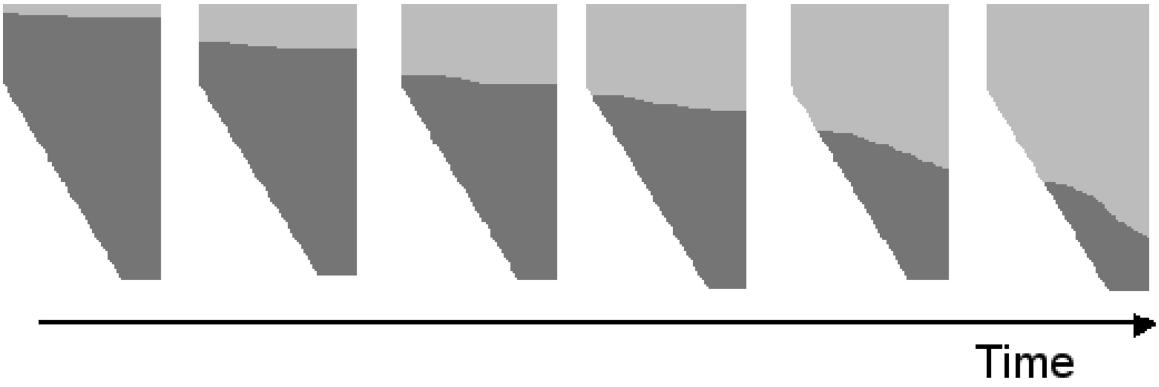

FIG. 6. Material interface profiles during hopper discharge.

The diffusive velocity was written as the product of a characteristic transport coefficient D_i, i.e. diffusion coefficient and the ith phase fraction gradient:

$$\underline{v}_i^D = -D_i \nabla f_i \tag{4}$$

where the negative sign indicated material motion down a fraction gradient. The drift velocity due to shear induced segregation was taken to be a function of the bulk velocity gradient:

$$\underline{v}_i^s = \frac{\eta_i}{|\underline{u}^b|}(\nabla(\underline{u}^b \cdot \underline{i}) + \nabla(\underline{u}^b \cdot \underline{j}) + \nabla(\underline{u}^b \cdot \underline{k})) \tag{5}$$

where η_i is a shear-induced segregation transport coefficient for the ith mixture component, $|\underline{u}^b|$ is the magnitude of the bulk velocity vector and $\underline{i}, \underline{j}, \underline{k}$ are the unit vectors in the x, y, z directions, respectively. There is no negative sign in equation 5, since strain driven segregation causes material to move up a gradient of bulk strain rate. Of the two processes, shear induced segregation is the trigger mechanism, based on bulk velocity gradients, which causes species separation and subsequent concentration gradients, with the coarse particles concentrating in regions of high-shear. Thus, diffusion is activated as a response mechanism, and causes fines to concentrate away from high-shear regions.

The percolation drift velocity is different to the other two velocities, since it is driven only by a body force, i.e. gravity, and does not depend on any thermodynamic property of the mixture. The feasibility of percolation is a function of the mixture composition and size ratio. Thus, for a binary mixture, the functional form employed was:

$$\underline{v}_i^p = K_i \epsilon \left(1 - \frac{d_i}{d_2}\right) \underline{g} \tag{6}$$

where K_i is the percolation coefficient, ϵ is the available voidage in the control volume, such that $\epsilon = 1 - f$, d_1 and d_2 are the particle diameters of the fines and coarse phases, respectively,

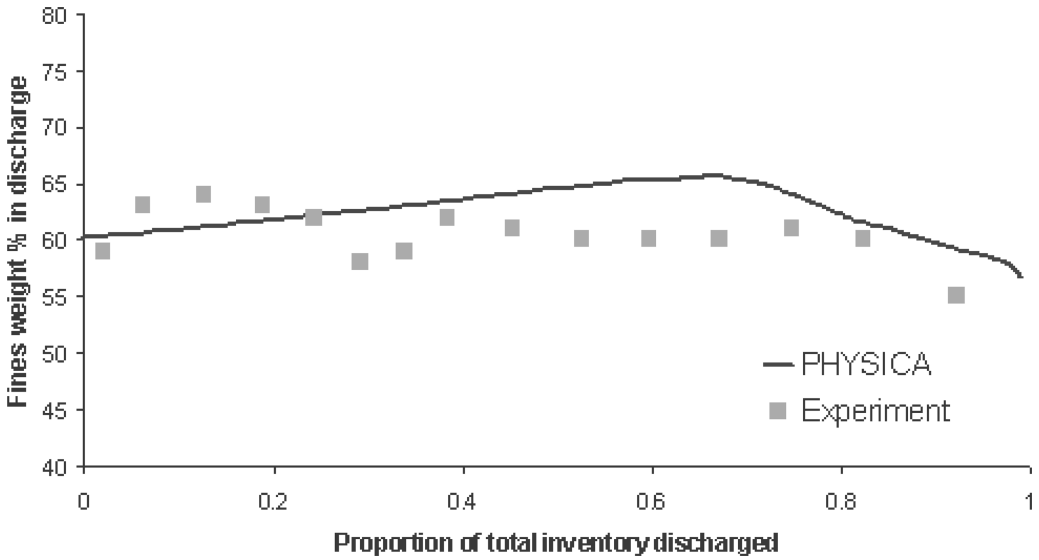

FIG. 7. Temporal variations in fines weight during hopper discharge.

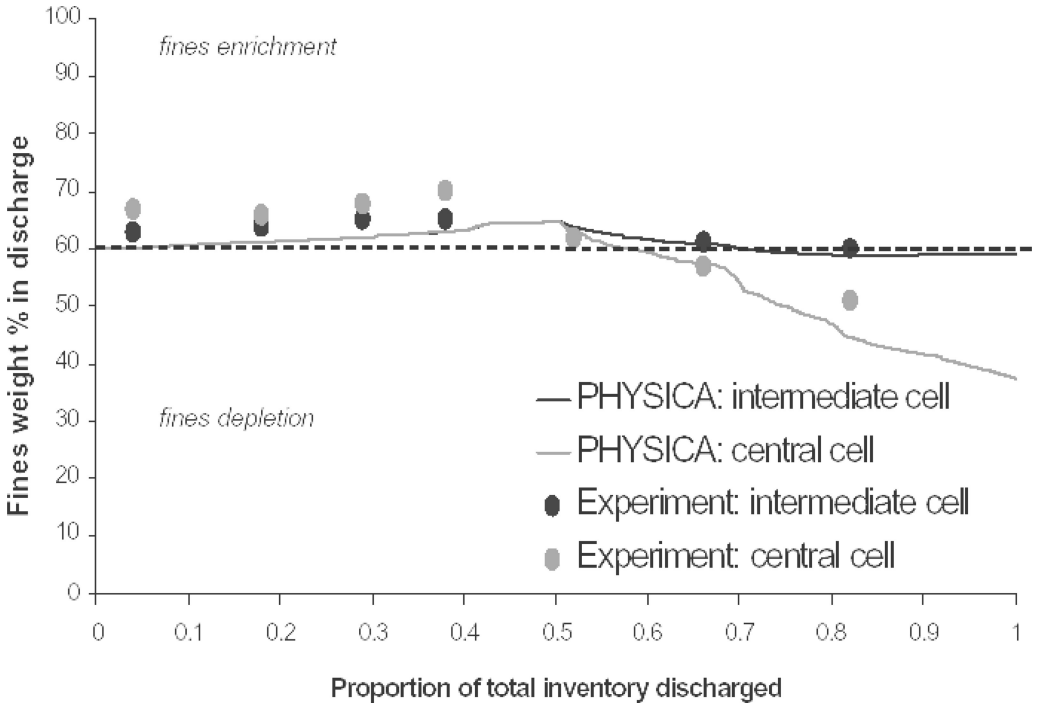

FIG. 8. Variation in fines weight.

and $\underline{g}$ is gravity. This indicated that percolation acted only if two neighboring volumes were along the line of action of gravity. It should also be noted that percolation drift velocities applied only to the fines phase, i.e. K_{coarse} was zero everywhere in the computational domain.

The transport coefficients D_i, η_i and K_i of equations 4, 5, 6 were calculated for each mixture phase in the micro-physical framework by using linear-response theory, which involved integration of the relevant time correlation functions [40].

This continuum granular flow model is implemented in the PHYSICA framework and has been used to investigate a range of process scenarios. The numerical model was tested for its consistency in representing, realistically, binary mixture flow patterns and was then used to simulate experimental data obtained during discharge under gravity of a binary mixture from a small mass-flow cylindrical hopper. For reasons of simplicity, and due to the observed symmetry of the flow around the central axis of the hopper for the simulated cases, semi-3D geometry was chosen, with a hopper slice of 5° angle being simulated.

The simulation was performed to test the model consistency. A 60-40 mixture was chosen, i.e. consisting of 60% fines and 40% coarse particles, uniformly distributed, of 2:1 particle size ratio, initial density of 950 kgm^{-3} and solids density of 2100 kgm^{-3} and was left to discharge under gravity from a hopper. The hopper's cylindrical section was 6.3 cm tall, its conical section was 7 cm tall, and its half-angle was 30°. The inlet diameter was 10.5 cm, while the outlet diameter was 2.5 cm. A sharp discontinuity in the mixture composition was assumed for a small slice of material around the center of the hopper. At this region, the material composition was assumed to consist of 95% fines and only 5% coarse particles. The transport coefficients were calculated for the two mixture phases in the micro-physical framework and were directly imported into the continuum frame work. Figure 6 shows the predicted profiles of the granular material as the hopper emptied and agrees well with the observations of a process behaving under mass flow [46,47].

Figure 7 and Figure 8 show the comparisons of the model with experimental data in the emptying of the hopper, where the transport coefficients were calculated in micro-physical framework. Figure 7 shows the time varying distribution of fines in the outflow that is due to segregation in the hopper, whilst Figure 8 shows the temporal variation at two locations in the hopper. In order to make these predictions it is vital to capture both the macroscopic behavior of the granular material as well as the local scale effects that influence the segregation of fine from coarse materials.

5. CONCLUSIONS

Given that simulation technology underwrites an increasing proportion of engineered products, then the demands upon its capability will grow inexorably to incorporate ever more precise physical details of processes and systems. This leads to demands for a greater capacity in representing the interactions amongst distinct phenomena at multiple length and time scales. It is now quite possible to conceive of strategies to represent such phenomena, but to do so requires software technologies that both incorporate the interactions and enable them to run on

HPPC systems, so that they can be run in practical simulation times.

In this paper one approach to the development of a core multi-physics simulation software technology is described and used on two problems that illustrate a range of the issues that need to be addressed in the multi-facetted aspects of this class of mathematical modelling.

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